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Applicability of the explainable machine learning techniques in surface Ozone simulation and formation sensitivity analysis

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Gaining insight into the response of surface ozone (O3) formation to its precursors, primarily nitrogen oxides (NOx) and volatile organic compounds (VOC), is still challenging due to the complex formation mechanisms involved.
The subject of this study concerns a methodology for analysing O3 sensitivity to NOx and VOC precursors. The approach is based on the Machine Learning (ML) techniques to identify the complex, non-linear relationships between input features and model output, combined with the Shapley additive explanation (SHAP) method to explore the impact of each feature on O3 concentrations.
To this end, a ML-XGBoost model has been developed to predict O3 concentrations based on hourly data of pollutants and meteorological parameters acquired during several years in an urban area. The SHAP approach has been applied to evaluate the main drivers explaining the changes in O3 predicted concentrations. Finally, the ML model has been applied to derive O3 formation sensitivity curves from measured data of VOC and NOx.
A range of findings have been identified in various seasonal contexts, demonstrating the efficacy of a ML model based on observational data in investigating the drivers of O3 formation. This knowledge is crucial for the effective management of O_3 pollution.

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